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New results, Directions and Opportunities

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Dynamics of supramolecular networks in hydrogen-bonded liquids

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Hydrogen bonds play a fundamental role for the fascinating properties of a large variety of materials, with molecular structures ranging from very complex, as bio-compounds, to relative simple, as water. At an intermediate level of complexity, monohydroxy alcohols form hydrogen-bonded networks which, due to their resistance against crystallization, can be investigated in a large dynamic range with various experimental techniques. At present, it is generally agreed upon that the alcohol networks are quasi-linear, however, no such a consensus exists regarding their microscopic dynamics. One debated issue is whether transient polymer-like structures are responsible for the appearance of the anomalously strong, slow, and exponential (Debye-like) dielectric process observed for these materials in addition to their structural relaxation [1]. Based on experimental results recently obtained for neat and diluted alcohols we will critically assess various microscopic models aiming at solving the long-standing puzzle surrounding the Debye process in hydrogen-bonded liquids [2,3].

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Invited talk

MA-8

Debye peak in molecular glass-forming liquids: Insights from molecular dynamics simulations

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In the framework of the glass transition phenomena, there has been recently revived interest for hydrogen-bonded (HB) liquids composed of molecules of low molecular weight. It well recognized from x-ray and neutron scattering experiments that primary alcohols and substituted aromatics HB liquids exhibit a small-Q peak of the structure factor S(Q), below the first sharp diffraction peak. Due to the strong directional hydrogen bonding, these liquids tend to be locally more organized than ordinary van der Waals liquids. The existence of this peak can thus be interpreted as the presence of some short range arrangements of nanometer scale. It is not totally clear about which shapes these HB aggregates come in. From broad band dielectric spectroscopy experiments, it was shown that some monohydroxy alcohols and drugs also exhibit a surprising relaxation corresponding to a purely Debye-type decay whose origin is not understood but could be related to hydrogen-bonded associations. Molecular dynamics simulations have been performed to shed some light on some dynamical properties of these liquids.

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